

The Small Polaron Crossover: Role of Dimensionality

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The crossover from quasi free electron to small polaron in the Holstein model for a single electron is studied by means of both exact and self-consistent calculations in one dimension and on an infinite coordination lattice, in order to understand the role of dimensionality in such a crossover. We show that a small polaron ground-state occurs when both strong coupling ($\lambda > 1$) and multiphonon ($\alpha^2 > 1$) conditions are fulfilled leading to different relevant coupling constants (λ) in adiabatic and (α^2) anti adiabatic region of the parameters space. We also show that the self-consistent calculations obtained by including the first electron-phonon vertex correction give accurate results in a sizeable region of the phase diagram well separated from the polaronic crossover.

I. INTRODUCTION

Recent optical measurements of the insulating parent compounds of the high-temperature superconductors show the presence of polaronic carriers [1], and evidence for intermediate and strong lattice distortions has been given also for the colossal magnetoresistance manganites [2] and Nickel compounds [3]. The recent observation of one-dimensional stripes in the high-temperature superconductors [4] and in manganites suggests a comprehensive study of the role of dimensionality in the polaronic crossover. A detailed study of the small polaron crossover is demanded also by the recent experimental results on manganites [5].

The polaronic state is characterized by strong local electron-lattice correlation and is a non-perturbative phenomenon. It therefore cannot be described by simple summation of the perturbative series such as the one which defines the Migdal-Eliashberg (ME) theory. Here, we provide a detailed study of the crossover which occurs at intermediate electron-lattice couplings from quasi-free electron to small polaron ground state, with a particular emphasis on the role of system dimensionality.

We consider the simple Holstein molecular-crystal Hamiltonian for a single electron, which reads:

$$\mathcal{H} = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + g \sum_i c_i^\dagger c_i (a_i + a_i^\dagger) + \omega_0 \sum_i a_i^\dagger a_i \quad (1)$$

where c_i (c_i^\dagger) and a_i (a_i^\dagger) are, respectively, the destruction (creation) operators for an electron and for a dispersionless phonon of frequency ω_0 on site i . The hamiltonian (1) represents a non-trivial many-body problem and it has been already studied in recent years by means of numerical [6–9] and analytical [10–12] techniques.

Two dimensionless parameters are introduced to measure the strength of electron-phonon (*el-ph*) interaction: $\lambda = g^2/(D\omega_0)$ and $\alpha = g/\omega_0$, where $D = 2td$ is the half-bandwidth for the free electron and d is the system dimensionality.

λ is originally introduced in the weak coupling perturbation theory ($g/t \ll 1$) and is the coupling parameter of a ME approach in the case of one electron. It can also be viewed as the ratio between the small polaron energy $E_p = -g^2/\omega_0$ and the free electron energy $E_{\text{free}} = -D$.

The parameter α is the relevant coupling in the *atomic limit* ($t = 0$). In this limit α measures the lattice displacement associated to the polaron and α^2 is the average number of phonons bound to the electron. According to the Lang-Firsov results followed by the Holstein approximation, α also rules the reduction of the effective hopping $t^* = t \exp(-\alpha^2)$ [9,13].

Besides λ and α , the *el-ph* system described by eq.(1) is governed also by another dimensionless parameter: ω_0/t . It measures the degree of adiabaticity of the lattice motion (lattice kinetic energy $\simeq \omega_0$) compared to the electron one (electron kinetic energy $\simeq t$). In the adiabatic regime ($\omega_0/t \ll 1$), $\lambda > 1$ is a condition sufficient to give a polaronic state since the electron is bound to the slowly moving lattice giving rise to a strong enhancement of effective mass. In the antiadiabatic regime ($\omega_0/t \gg 1$) such a picture is no longer true due to the fast lattice motion. In this case, polaronic features such as strong local electron-lattice correlations arise only when the electron is bound to a *large* number of phonons ($\alpha^2 > 1$). To summarize, in both adiabatic and antiadiabatic regimes, a polaronic state is formed when *both* $\lambda > 1$ and $\alpha^2 > 1$ inequalities are fulfilled [9]. This conclusion is in contrast with ref. [10] where it is argued that $\lambda > 1$ is the only condition for small polaron formation.

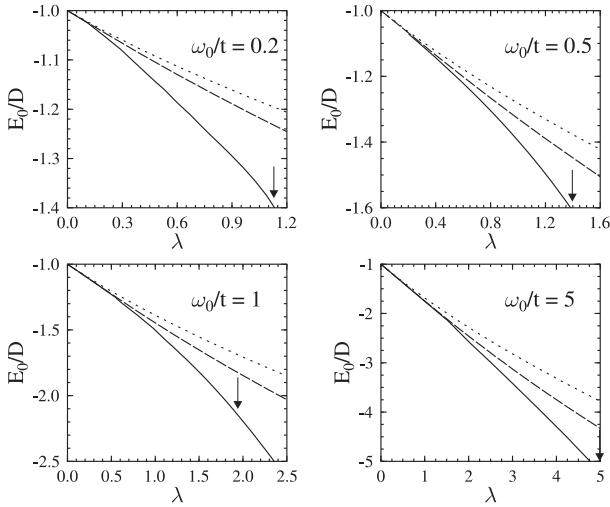


FIG. 1. Ground state energy results in $d=1$. The exact diagonalization results are compared with the NCA (short dashed) and VCA (long dashed) calculations. The arrows mark λ_c (see Fig.3).

The parameter ω_0/t influences also the dependence of the *el-ph* coupled system on the system dimensionality. We shall show that in the antiadiabatic regime the small polaron formation does not depend on the system dimensionality. On the other hand, dimensionality plays a crucial role in the adiabatic regime $\omega_0 \ll t$. This can be traced back to the adiabatic limit $\omega_0/t = 0$. In fact, in $d=1$ the ground state is localized for any finite value of λ and a crossover occurs between *large* and *small* polaron at $\lambda \simeq 1$, whereas for $d \geq 2$ it has been shown that a localization transition occurs at finite λ from free electron to small polaron [14]. The different adiabatic behaviors between 1d and 2d systems could be relevant to describe the motion of polarons as defects on top of 1d charge striped structures such as those observed in cuprates [4] and manganites [2].

II. RESULTS

We study the relevance of ω_0/t and of the lattice dimensionality d by using two alternative exact calculations: exact diagonalization of small one dimensional clusters (ED-1d) and dynamical mean field theory (DMFT-3d). In the ED-1d approach, the infinite phonon Hilbert space must be truncated to allow for a given maximum number of phonons per site n_{max} . In order to properly describe the multiphonon regime (especially in the adiabatic regime where a large number of low energy phonons can be excited) we chose a cut-off of $n_{\text{max}} = 20$. This high value forced us to restrict our analysis to a four-site cluster in the strong-coupling adiabatic regime.

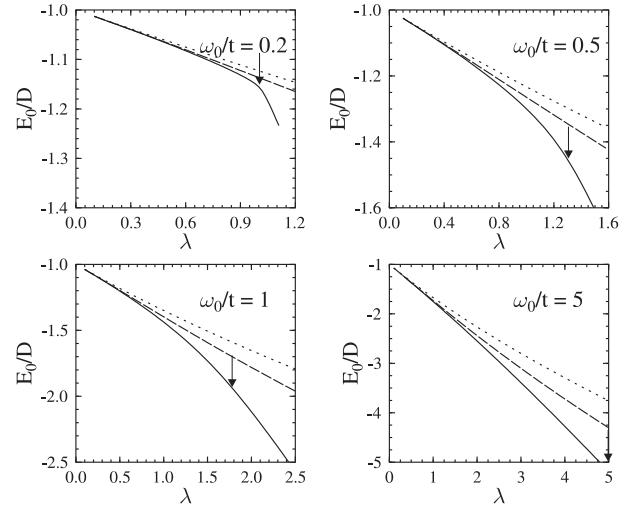


FIG. 2. Ground state energy results for an infinite coordination lattice. Comparison between dynamical mean field (solid line), NCA (short dashed) and VCA (long dashed). The arrows mark λ_c (see Fig.3).

In the weak-coupling regime and for larger phonon frequencies a lower value of n_{max} is needed, allowing us to consider larger clusters up to ten-twelve sites. We checked that finite-size effects do not affect the crossover coupling, since small-polaron formation is a local, high energy process.

The dynamical mean field theory approach can be seen as the exact solution of the small polaron problem on an infinite coordination lattice [11]. The formulation of the DMFT requires the knowledge of the free particle DOS. A semi-circular DOS can mimic a three-dimensional case: in the following we will therefore refer to this approach to as DMFT-3d.

We calculate the exact ground state energy E_0 obtained by means of ED-1d and DMFT-3d and we compare the results with the self-consistent non-crossing (NCA) and vertex corrected approximations (VCA). These two approximations are defined by the self-consistent calculation of the electronic zero-temperature self-energy $\Sigma(k, \omega)$ given below:

$$\Sigma(k, \omega) = \frac{2\lambda\omega_0 t}{N} \sum_p G(p, \omega - \omega_0) \times \left[1 + \frac{2\lambda\omega_0 t}{N} \sum_q G(q - p + k, \omega - \omega_0) G(q, \omega - 2\omega_0) \right], \quad (2)$$

where $G(k, \omega)$ is the retarded fully renormalized single electron Green's function:

$$G(k, \omega)^{-1} = \omega - \epsilon_k - \Sigma(k, \omega) + i\delta. \quad (3)$$

which will be determined self-consistently. From eqs.(2,3), the ground state energy E_0 is given by the lowest energy solution of $\text{Re } G(k, E_0)^{-1} = 0$. The NCA approach amounts to compute Σ by retaining only the 1 in the square brackets of eq. (2). The VCA is instead given

by the inclusion also of the second term in square brackets of eq.(2) which represents the first vertex correction. This approach is formally similar to the approximation scheme used in the formulation of the non-adiabatic theory of superconductivity [15] and a comparison with exact results therefore provides also a test of reliability of such an approach for the one-electron case.

In fig.1 we compare the ground-state energy E_0 obtained by ED-1d with the NCA and VCA results. The same quantities evaluated in the DMFT-3d case are shown in fig. 2. We have chosen the same half-bandwidth D in both DMFT-3d and ED-1d. In the adiabatic regime, the agreement of both approximations with exact results strongly depends on the system dimensionality as a result of the different low-energy behaviour of the DOS . In fact, moving from $\omega_0/t = 0.2$ to $\omega_0/t = 0.5$, before the crossover the agreement of the self-consistent calculations with the exact results is improved for the 1d case (fig. 1) whereas it becomes poorer for the 3d one (fig. 2). However, the VCA approach represents a significative improvement with respect to the NCA for every system dimensionality and over a significant range of parameters.

As it is seen from the comparison of fig. 1 and 2, for large ω_0/t both approximate and exact results tend to become independent of dimensionality. This can be understood by realizing that in this regime the system can be thought as a flat band “atomic” system in interaction with high energy phonons. It is also clear from figs. 1 and 2 that both the self-consistent NCA and VCA calculations deviate from the exact results when the crossover towards the small polaron regime is approached.

A complete comparison between the exact results and the VCA approach in the parameter space $\lambda-\omega_0/t$ is shown in figs. 3(a)-(b). We explicitly evaluated both in 1d (a) and 3d (b) the relative difference $\delta E_0 = 2|E_0^{\text{VCA}} - E_0^{\text{exact}}|/|E_0^{\text{VCA}} + E_0^{\text{exact}}|$ where E_0^{exact} and E_0^{VCA} are the ground-state energies evaluated by exact techniques and the VCA, respectively. To analyze the region in the parameter space where the VCA agrees within a given accuracy with the exact results we report in figs. 3(a)-(b) lines of constant δE_0 .

As already mentioned, the agreement between self-consistent approximations and exact results is sensible to dimensionality. For $d > 2$, approaching the adiabatic limit and for small couplings the electron tends to be free. For this reason self-consistent approximations work well. On the contrary, in the adiabatic limit and for $d=1$ the ground state is a localized large polaron and self-consistent approximations fail to predict its energy. In general, VCA (and so NCA) works well outside the polaron region whatever polarons are either small or large. This can be seen directly from figs. 3(a)-(b) where the critical coupling λ_c of the crossover to small polaron is depicted as a dotted line. The critical coupling λ_c is defined as the value at which dE_0/dg has maximum slope.

In the same figures, we provide also an estimate of the width of the crossover (shaded areas) obtained by looking at the maximum slope of $|d^2E_0/dg^2|$. We checked that different criteria, like *e.g.* the effective mass enhancement [11], provide the same qualitative results.

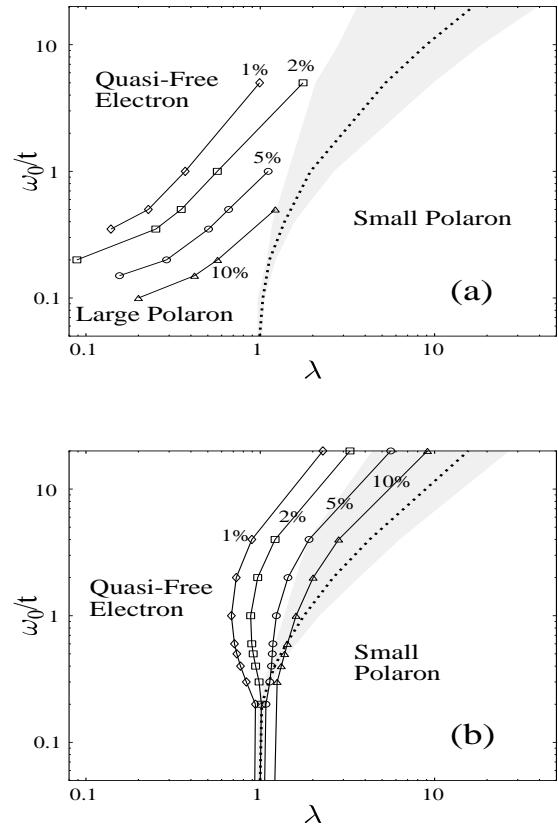


FIG. 3. Phase diagram in the $\lambda-\omega_0/t$ plane for the one-dimensional (a) and the infinite coordination lattice (b) Holstein model. The dotted line is the polaron crossover value λ_c and the width of the crossover is evidenced by a shaded area. The isolines represent the relative difference between the exact and the VCA result for the ground state energy (see text).

III. CONCLUSIONS

In conclusion, we have shown that the crossover towards the small polaron state depends strongly on the adiabaticity parameter ω_0/t . In the antiadiabatic regime the crossover is ruled by α^2 and it is independent of the system dimensionality. In the adiabatic regime the relevant coupling is λ and the crossover occurs from large to small polaron in 1d, while in 3d the crossover is from quasi free electrons to small polarons. In the latter case

self-consistent approximations work better than in 1d systems. We have also shown that self-consistent calculations provide ground state energies which agree well with exact results outside the small and large polaron region of the phase diagram and that such an agreement is increased when vertex corrections are taken into account.

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